

Is Quantization of QCD Unique at the Non-Perturbative Level ?

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We find that QCD in covariant gauge yields zero for the topological susceptibility, even at the nonperturbative level. The result is derived in two ways, one using translational invariance, and the other using the BRST Hamiltonian. Comparison with the canonical formalism suggests that QCD is not uniquely defined at the nonperturbative level. Supporting evidence is also provided in 1+1 dimensions. Our results imply that the strong CP problem admits a trivial resolution in covariant gauge, but obstacles remain for the U(1) problem.

1. QCD is currently by far the favored theory of strong interactions. At the perturbative level, it fares well : the theory is well defined and agrees with experiment. The situation is less satisfactory at the non-perturbative level. Besides the well-known problems of demonstrating confinement and chiral symmetry breaking, there is a growing body of evidence that the theory is not uniquely defined at the non-perturbative level. First, dimensional transmutation implies that the QCD perturbation series is not Borel summable, so the series does not uniquely define the theory. The Gribov ambiguity [1] opens the possibility that covariant and canonical quantization are inequivalent. This note adds another piece of evidence : BRST quantization implies that physics is automatically independent of the vacuum angle θ , in contrast with the canonical formalism. In particular, the topological susceptibility χ is identically zero in covariant gauge, which has significant consequences for the U(1) problem. Evidence for a non-unique θ dependence is also found in 1+1 dimensions.

2. It is simple to see that χ is zero in covariant gauge [2]. As well known, the topological term in the QCD Lagrangian $\theta \Xi$ is a total divergence,

$$\Xi = (g^2/32\pi^2) F_{\mu\nu}^a \tilde{F}^{\mu\nu a} = \partial^\mu K_\mu \quad (1)$$

where

$$K_\mu = \frac{g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} (A^{\nu a} F^{\rho\sigma a} - \frac{g}{3} f^{abc} A^{\nu a} A^{\rho b} A^{\sigma c}) \quad (2)$$

is the Loos-Chern-Simons current [3]. In covariant gauge

$$\begin{aligned} \langle \theta | K_\mu(x) | \theta \rangle &= \langle \theta | e^{iP \cdot x} K_\mu(0) e^{-iP \cdot x} | \theta \rangle \\ &= \langle \theta | K_\mu(0) | \theta \rangle \end{aligned} \quad (3)$$

is constant (just as for the Higgs field), where $|\theta\rangle$ are the θ vacua and P_μ is the energy-momentum operator.

Hence, $\langle \theta | \Xi | \theta \rangle = \partial^\mu \langle \theta | K_\mu | \theta \rangle = 0$ for any θ , and $\chi = \partial < \theta | \Xi | \theta \rangle / \partial \theta = 0$ as well.

It is important that the derivation fails to go through in the canonical formalism. The vacuum state then obeys Gauss' law, so the vacuum expectation value $\langle K_\mu \rangle_\theta$ is ambiguous like $\langle x \rangle_p$ in quantum mechanics. However, no such ambiguity exists in covariant gauge. Since θ can be taken as a coupling constant, the so-called θ superselection rule trivially operates and a single Hilbert space suffices to describe physics for fixed θ , including gauge-variant operators. This space has indefinite metric, so one must further construct the physical Hilbert space out of it [4]. Nevertheless, as familiar since Gupta and Bleuler, the norm of the vacuum state in the original Hilbert space is equal to the norm in the physical Hilbert space, which is one. Hence $|\theta\rangle$ is a proper element of the original Hilbert space, and $\langle \theta | K_\mu | \theta \rangle$ is well defined.

Our analysis applies to any formulation of QCD where the vacuum expectation value of a gauge-variant operator is well-defined and translation invariant.

3. The previous result may also be derived by another argument which is more formal but yields stronger results as well as some new insight.

In classical theory, adding a total divergence to the Lagrangian does not affect the physics, since the equations of motion are unchanged. However, this does not mean that the Hamiltonian remains the same; rather it undergoes a canonical transformation.

Similarly, the BRST Hamiltonian for different vacuum angles is related by a unitary transformation $H(\theta) = e^{i\theta \mathbf{X}} H(0) e^{-i\theta \mathbf{X}}$ where $\mathbf{X} = \int d^3x K_0$. This may be explicitly checked in covariant gauge, or in general derived from the quantum action principle,

$$\delta_\theta \langle 2 | 1 \rangle = i \delta \theta \langle 2 | (\mathbf{X}(2) - \mathbf{X}(1)) | 1 \rangle \quad (4)$$

where 1, 2 refer to spacelike hypersurfaces. In the former case, one must make sure to write the Hamiltonian in terms of canonical variables [5].

The question therefore is whether unitarily equivalent Hamiltonians can give inequivalent physics.

Let $|0\rangle$ be the physical ground state of $H(0)$ in the BRST formalism. It must obey [4]

$$H(0)|0\rangle = 0 \quad \mathbf{Q}_{\text{BRST}}|0\rangle = 0 \quad (5)$$

where \mathbf{Q}_{BRST} is the BRST charge. Since \mathbf{X} is invariant under infinitesimal gauge transformations, it is invariant under BRST transformations. Hence,

$$H(\theta)e^{i\theta\mathbf{X}}|0\rangle = 0 \quad \mathbf{Q}_{\text{BRST}}e^{i\theta\mathbf{X}}|0\rangle = 0 \quad (6)$$

which means that $e^{i\theta\mathbf{X}}|0\rangle$ is the physical ground state of $H(\theta)$ with the same energy. The θ -independence of the vacuum energy density \mathcal{E} implies that $\chi = -\partial^2\mathcal{E}/\partial\theta^2 = 0$ as before.

A further consequence is that strong CP violation is absent in the BRST formalism for any value of θ , provided it is absent for $\theta = 0$. If $\text{CP}(0)$ commutes with $H(0)$ and \mathbf{Q}_{BRST} with $\text{CP}(0)|0\rangle = |0\rangle$, then $\text{CP}(\theta) = e^{i\theta\mathbf{X}}\text{CP}(0)e^{-i\theta\mathbf{X}}$ commutes with $H(\theta)$ and \mathbf{Q}_{BRST} , with $\text{CP}(\theta)e^{i\theta\mathbf{X}}|0\rangle = e^{i\theta\mathbf{X}}|0\rangle$. It is easy to extend these arguments to show that $H(\theta)$ is physically equivalent to $H(0)$ in the BRST formalism. The physical states and observables are in one-to-one correspondence, and the matrix elements are the same.

The results may again be contrasted with the canonical formalism. The Hamiltonian then still has the structure $H(\theta) = e^{i\theta\mathbf{X}}H(0)e^{-i\theta\mathbf{X}}$, but the subsidiary condition is altered to [6]

$$\mathbf{U}[\Omega]|\text{phys}\rangle = |\text{phys}\rangle \quad (7)$$

where $\mathbf{U}[\Omega]$ is the operator implementing the proper gauge transformation Ω . If Ω is ‘large’, \mathbf{X} is shifted and $e^{i\theta\mathbf{X}}|0\rangle$ is no longer a physical state unless θ is an integer multiple of 2π . Hence, Hamiltonians with different θ are generally expected to be inequivalent modulo 2π . This is in agreement with the general wisdom, although we are unaware of any explicit calculations for QCD in the canonical formalism [7].

4. The Hamiltonian analysis above suggests that the source of the probable inequivalence is that BRST invariance

$$\mathbf{Q}_{\text{BRST}}|\text{phys}\rangle = 0 \quad (8)$$

mimics Gauss’ law, but not invariance under ‘large’ gauge transformations. As a check, QED is independent of θ , since there are no ‘large’ gauge transformations. Also in the Polyakov model [8], the analogue of \mathbf{X} is fully gauge invariant, so it commutes with either constraints (7) or (8). It follows that physics is again independent of θ , in agreement with explicit computation [9].

Let us therefore entertain the possibility that the BRST formalism for QCD is missing some extra constraints. First, it will not do to simply impose (7) with ‘large’ Ω in the BRST formalism. The BRST Hamiltonian is not invariant under ordinary gauge transformations, so the new constraint will not be preserved under time evolution. Furthermore, an extra constraint would not help as far as covariant gauge is concerned. The vacuum would remain normalizable and translational invariant, so $\langle\theta|\Xi|\theta\rangle$ would remain zero by (3).

A different approach is to replace (5) by the weaker condition

$$H(0)|0\rangle = \mathbf{Q}_{\text{BRST}}|\Lambda\rangle \quad \mathbf{Q}_{\text{BRST}}|0\rangle = 0 \quad (9)$$

where $|\Lambda\rangle$ is some vector. However, this upsets translational invariance for the vacuum expectation value of gauge-variant operators, so the resulting formalism is no longer covariant gauge.

The above arguments do not completely rule the possibility that a suitable modification of the BRST formalism may bring it in line with the canonical formalism. However, the arguments are sufficient to show that our basic result will remain unaltered. Covariant gauge gives $\langle\theta|\Xi|\theta\rangle = 0$, even if the other (yet hypothetical) formalism gives $\langle\theta|\Xi|\theta\rangle \neq 0$.

5. Our analysis has revealed the strong likelihood that covariant quantization of QCD is inequivalent to canonical quantization, except perhaps with massless quarks. If both schemes lead to consistent theories, it means that QCD is not uniquely defined at the non-perturbative level.

In hindsight, the situation is not totally unexpected. We know of no way at present to show that the two quantization schemes are equivalent. As mentioned in the beginning, the QCD perturbation series does not uniquely define the theory. Feynman’s one-loop equivalence was extended to all orders by DeWitt [10]. However, the proof relies on asymptotic fields (free quarks and gluons), so it is unlikely to extend to the non-perturbative regime. Mandelstam’s proof [11] was given before the Gribov ambiguity was discovered, so it does not take it into account. As well known, the Gribov ambiguity also spoils the Faddeev-Popov prescription except in some special cases [12]. Also, recent investigations [13] show that the application of the Batalin-Fradkin-Vilkovitsky theorem has its own shortcomings in the presence of the Gribov ambiguity.

In the last case in fact, BRST quantization has been shown to be inequivalent to Dirac quantization for certain models. The models, however, are quantum mechanical and do not have a topological term. In the following, we treat a gauge theory with a topological term, where the inequivalence between covariant and canonical quantization can be explicitly seen.

6. The theory is free electromagnetism in 1+1 dimensions, where ‘large’ gauge invariance is imposed in the canonical formalism, and a Fermi-type condition is used for covariant gauge. The analog of Ξ is the electric field F_{01} . For dimensional reasons, we normalize $\Xi = eF_{01}/2\pi$ so that $\mathbf{X} = (e/2\pi)\int dx^1 A_1(x)$, where e is a non-zero parameter with the dimensions of charge (mass).

Gauge invariant quantization gives Maxwell equations $\partial_\mu F_{01} = 0$ as operator relations, so F_{01} is a constant. This is compatible with the commutation relation

$$[F_{\alpha\beta}(x), F_{\mu\nu}(y)] = ig_{\beta\nu}\partial_\alpha\partial_\mu D(x-y) \pm 3 \text{ permutations} \quad (10)$$

since the right hand side vanishes in 1+1 dimensions.

Canonical Quantization. In the $A_0 = 0$ gauge, the Lagrangian is

$$\mathcal{L}_{can} = \frac{1}{2}(\partial_0 A^1)^2 - \frac{e\theta}{2\pi} \partial_0 A^1 \quad (11)$$

The canonical conjugate of A_1 is $\Pi = -F_{01} - (e\theta)/2\pi$ and the Hamiltonian is

$$H = \int dx^1 \frac{1}{2} \left(\Pi + \left(\frac{e\theta}{2\pi} \right) \right)^2 = \int dx^1 \frac{1}{2} (F_{01})^2 \quad (12)$$

The theory remains invariant under time-independent gauge transformations

$$A_1(t, x) \rightarrow A_1(t, x) + \frac{1}{e} \lambda'(x) \quad (13)$$

generated by

$$\mathbf{G}[\lambda] = \frac{1}{e} \int dx \lambda'(x) \Pi(t, x) \quad (14)$$

in order that the transformations do not change the physical state, $\Omega(x) = e^{i\lambda(x)}$ must approach one at infinity. The winding number

$$\begin{aligned} w[\Omega] &= -\frac{i}{2\pi} \int dx \Omega^\dagger(x) \Omega'(x) \\ &= +\frac{1}{2\pi} (\lambda(+\infty) - \lambda(-\infty)) \end{aligned} \quad (15)$$

is then an integer and $\mathbf{X} = e \int dx A_1(t, x)/2\pi$ transforms as $\mathbf{X} \rightarrow \mathbf{X} + w[\Omega]$. We note that the theory has acquired another gauge-invariant dynamical variable $e^{i2\pi\mathbf{X}}$ besides the electric field.

The residual gauge-invariance (13) implies that a constraint must be imposed. Since the right hand side of (13) is $e^{-i\mathbf{G}[\lambda]} A_1(t, x) e^{i\mathbf{G}[\lambda]}$, the desired constraint is

$$e^{i\mathbf{G}[\lambda]} |\text{phys}\rangle = |\text{phys}\rangle \quad (16)$$

where λ is a gauge function with integer winding number, so that physical states are invariant under both ‘small’ and ‘large’ gauge transformations. Since the electric field F_{01} , the Hamiltonian (12), and the constraint $e^{i\mathbf{G}[\lambda]}$ commute, it is easy to determine the physical spectrum. The eigenstate $F_{01}(x)|\theta\rangle = -(e\theta/2\pi)|\theta\rangle$ is the physical ground state for $|\theta| < \pi$. For $\theta = \pm\pi$, there is a twofold degeneracy induced by $e^{\pm 2\pi i\mathbf{X}}$, and the structure repeats itself with a period 2π .

On the other hand, if λ is restricted to have zero winding number in (16), $F_{01} = 0$ is the ground state spectrum for each θ . Evidently, ‘large’ gauge invariance makes a difference. This concludes canonical quantization.

Covariant Quantization. In covariant gauge, the Lagrangian is

$$\mathcal{L}_{cov} = \frac{1}{2}(F_{01})^2 + \frac{e\theta}{2\pi} F_{01} + \frac{\alpha}{2} b^2 + b \partial_\mu A^\mu \quad (17)$$

The canonical pairs are (A^0, b) and $(A^1, \Pi) = (A^1, -F_{01} - (e\theta/2\pi))$ and the Hamiltonian is

$$H = \int dx^1 \left(\frac{1}{2} \left(\Pi + \left(\frac{e\theta}{2\pi} \right) \right)^2 + A^0 \partial_1 \Pi - \frac{\alpha}{2} b^2 - b \partial_1 A^1 \right) \quad (18)$$

One must also choose between the Fermi-type condition $b(x)|\text{phys}\rangle = 0$ and the Gupta-Bleuler-type condition $b^+(x)|\text{phys}\rangle = 0$. Both are acceptable for local observables since $[b(x), F_{01}(y)] = [b^+(x), F_{01}(y)] = 0$. However, the Wightman function $\langle A_\mu(x) A_\nu(y) \rangle_{\text{conn}}$ is ill-defined with the Gupta-Bleuler condition, owing to infrared divergences peculiar to 1+1 dimensions. Since the vacuum $|\theta\rangle$ is normalizable, this means that A_μ is not well-defined as a quantum field.

If we choose the Fermi-type condition, the equations of motion

$$\begin{aligned} \partial_\mu F^{\mu\nu} &= \partial^\nu b \\ \square b &= 0 \end{aligned} \quad (19)$$

imply that the constraint is equivalent to

$$\begin{aligned} b(0, x)|\text{phys}\rangle &= 0 \\ \partial_1 \Pi(0, x)|\text{phys}\rangle &= 0 \end{aligned} \quad (20)$$

In this form it is clear that physical states are non-normalizable, so our translational argument does not go through. However, the very definition of field operators as (tempered) distributions implies that the second equation in (20) is equivalent to

$$\int dx \Lambda'(x) \Pi(0, x) |\text{phys}\rangle = 0 \quad (21)$$

where the function $\Lambda(x)$ must fall off at infinity. Hence ‘large’ gauge invariance is not included, and the physical ground state spectrum is $F_{01} = b = 0$ for each θ .

That θ does not affect the physics in general, may be demonstrated just as in section 3. The Hamiltonian (18) for different vacuum angles is related by $H(\theta) = e^{i\theta\mathbf{X}} H(0) e^{-i\theta\mathbf{X}}$. Also \mathbf{X} commutes with the constraint (20) at equal times $[\mathbf{X}(t), b(t, x)] = [\mathbf{X}(t), \partial_1 \Pi(t, x)] = 0$ hence all times.

In general, observables $\mathbf{Q}(\theta) = e^{i\theta\mathbf{X}} \mathbf{Q}(0) e^{-i\theta\mathbf{X}}$ and physical states $e^{i\theta\mathbf{X}} |\text{phys}_0\rangle$ are in one-to-one correspondence, and the matrix elements are the same, so physics is independent of θ in covariant gauge. As before, $H(\theta) = e^{i\theta\mathbf{X}} H(0) e^{-i\theta\mathbf{X}}$ in the canonical formalism also, but the proof does not go through there, since $e^{i\theta\mathbf{X}}$ does not commute with the ‘large’ gauge constraint (16) unless θ is an integer multiple of 2π .

Summary. It is interesting that covariant and canonical quantization are inequivalent, even though there is no Gribov ambiguity (at least in Euclidean space). However, this may be deceptive. Path integrals for gauge theories remain undefined formal objects if only the fields and the action \mathbf{I} are given. For QED in covariant gauge $\int [dA^\mu][db][d\psi][d\bar{\psi}] e^{i\mathbf{I}}$ does not distinguish whether Fermi or Gupta-Bleuler-type conditions are imposed. Similarly,

if we take $\mathbf{I} = \int d^2x \mathcal{L}_{\text{can}}$ of (16), $\int [dA^1] e^{i\mathbf{I}}$ does not incorporate the constraint (20). If we put in boundary conditions or delta functionals to specify the precise measure, we expect a Gribov-like obstacle in going from the canonical path integral to the covariant path integral.

In any case, we see clearly how the constraints matters. Furthermore, lack of ‘large’ gauge invariance does not imply lack of consistency. We conclude that all the arguments point consistently in the direction that QCD is generally non-unique at the non-perturbative level.

As for models, such as the the Schwinger model, the electroweak theory, or quantum gravity, we hope to discuss them in the future.

7. If strong CP violation can be trivially solved in covariant gauge, it is natural to ask what our results have to say for the U(1) problem. Let us briefly recall what the problem is and the various attempts to its solution. The axial U(1) symmetry of the QCD action is not apparent in nature, although a non-vanishing quark condensate suggests the existence of a ninth Nambu-Goldstone mode in the chiral limit [14]. This is known as the U(1) problem. The absence of such a mode in the hadronic spectrum is believed to be related to the chiral anomaly [15]. Based on the massless Schwinger model, Kogut and Susskind [16] suggested that quark confinement solves the problem. Their idea was further taken up by Weinberg [17] and others [4]. With the discovery of instantons, ‘t Hooft [18] has suggested that they may provide a solution to the problem through the anomaly, but this has been challenged by Crewther [21]. Witten [5] has proposed that the problem can be solved in the large N_c (number of colors) limit, where the anomaly can be treated as a perturbation. Witten’s proposal was later interpreted by Veneziano [20] in terms of vector ghosts. Much of this discussion has been carried out using covariant gauge.

Fortunately, we only need a double Ward identity [21] to make our point. With N_f flavors of quarks with equal mass m for simplicity, the identity reads

$$0 = -2i \langle \theta | \bar{q} q | \theta \rangle + 2i \frac{N_f^2}{m} \chi + 2m \int d^4x \langle \theta | T^* \bar{q} i \gamma_5 q(x) \bar{q} i \gamma_5 q(0) | \theta \rangle_{\text{conn}} \quad (22)$$

On the other hand, the absence of massless pseudoscalars for $m \neq 0$ in the flavor non-singlet channel gives

$$\begin{aligned} 0 &= \int d^4x \partial^\mu \langle \theta | T^* \bar{q} \gamma_\mu \gamma_5 \frac{\lambda^a}{2} q(x) \bar{q} i \gamma_5 \lambda^b q(0) | \theta \rangle \\ &= -\frac{i}{2} \langle \theta | \bar{q} [\lambda^a, \lambda^b]_+ q | \theta \rangle \\ &\quad + m \int d^4x \langle \theta | T^* \bar{q} i \gamma_5 \lambda^a q(x) \bar{q} i \gamma_5 \lambda^b q(0) | \theta \rangle_{\text{conn}} \quad (23) \end{aligned}$$

If $\chi = 0$ as in covariant gauge, (22) and (23) are essentially similar, and the same assumptions which imply the existence of Goldstone modes in the non-singlet channel

as $m \rightarrow 0$ also imply the existence of a physical U(1) Goldstone mode as $m \rightarrow 0$.

One may object that the flavor singlet channel can mix with glueballs, whereas the non-singlet channel cannot, so the assumptions need not be the same. However, if $\chi = 0$ and $\langle \theta | \bar{q} q | \theta \rangle \neq 0$, the zero momentum propagator $\int d^4x \langle \theta | T^* \bar{q} i \gamma_5 q(x) \bar{q} i \gamma_5 q(0) | \theta \rangle_{\text{conn}}$ must become singular as $m \rightarrow 0$. Glueballs cannot generate such a singularity unless their masses also go to zero as $m \rightarrow 0$. Massless glueballs are as bad as U(1) Goldstone modes.

To summarize, our results do not fundamentally alter the well-known trade-off between the U(1) problem and strong CP violation. If anything, they emphasize it further.

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Appendix. In this short Appendix, we would like to make some notes on n-vacua and normalizability. If we start out from n-vacua, the norm of the θ vacua is infinite as $\langle \theta | \theta \rangle = \sum_n 1$. However, the n-vacua violate the superselection rule and cluster decomposition. Furthermore, the divergence is merely the volume of the symmetry group, and may be factored out by a suitable choice of the configuration space. For example, a quantum mechanical system on the real line with a periodic potential $V(x+L) = V(x)$ is equivalent to a collection of systems on the interval $[0, L]$ with boundary conditions on the energy eigenfunctions $\psi(L) - e^{ikL} \psi(0) = \psi'(L) - e^{ikL} \psi'(0) = 0$. In the latter formulation, the ground state is normalizable for a given k . (As a toy model for vacuum tunneling, k corresponds to θ .)

Similarly, the natural configuration space of pure Yang-Mills theory in the canonical formalism is $\mathcal{A}^3/\mathcal{G}^3$, where \mathcal{A}^3 is the space of (three) vector potentials $A_i^a(\vec{x})$ and \mathcal{G}^3 is the group of proper gauge transformations $\Omega(\vec{x}) \rightarrow \mathbf{1}$ with $|\vec{x}| \rightarrow \infty$. The classical vacuum must obey $F_{ij}^a(x) = 0$. Again, all the n-vacua are identical in the classical limit, since \mathcal{G}^3 contains ‘large’ as well as ‘small’ gauge transformations. Instantons appear as non-contractible loops passing through the classical vacuum, corresponding to the fundamental group $\pi_1(\mathcal{A}^3/\mathcal{G}^3) = \mathbb{Z}$. Wave-functionals on $\mathcal{A}^3/\mathcal{G}^3$ directly constitute the physical Hilbert space, so the vacuum functional has unit norm by axiomatics. However, $\langle \theta | K_\mu | \theta \rangle$ remains ill-defined, since K_μ is not well-defined over $\mathcal{A}^3/\mathcal{G}^3$.

The conventional description based on n-vacua corresponds to taking the configuration space as $\mathcal{A}^3/\mathcal{G}_0^3$, where \mathcal{G}_0^3 is the group of ‘small’ gauge transformations. Physical wave-functionals must then be invariant under ‘large’ gauge transformations, so their norm is infinite.

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